Title: Integration of GRANTA MI with engineering analysis models

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Integration of GRANTA MI with engineering analysis models

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Prologue

- We should care about material data management (a.k.a. 'Granta') because we are both:
  - Producers of data: Calibrated Material Models (CMMs)
  - Consumers of data: Test data to calibrate CMMs
- NNSA cares about Granta now more than ever
  - They bought licenses for the whole complex ($1.5M)
    - They want to see these licenses used
  - They are paying for a shared classified Granta instance
  - They are mandating Granta use for some projects (e.g. Additive Manufacturing)

- **We should take advantage of NNSA's support by**:
  - Including Granta in work packages (e.g. to improve our CMM records in Granta)
  - Asking data producers to manage test data in Granta

Agenda

1. End state – planned Granta implementation across NSE
2. Current state – where we are compared to the end state
3. To-do – what we need to do to move closer to the end state
4. Deep dive – uncertainty quantification of CMM parameters in Granta

Emphasis is on Granta for CMMs

End state: Granta will be the trusted source for material data related to product definition and simulation
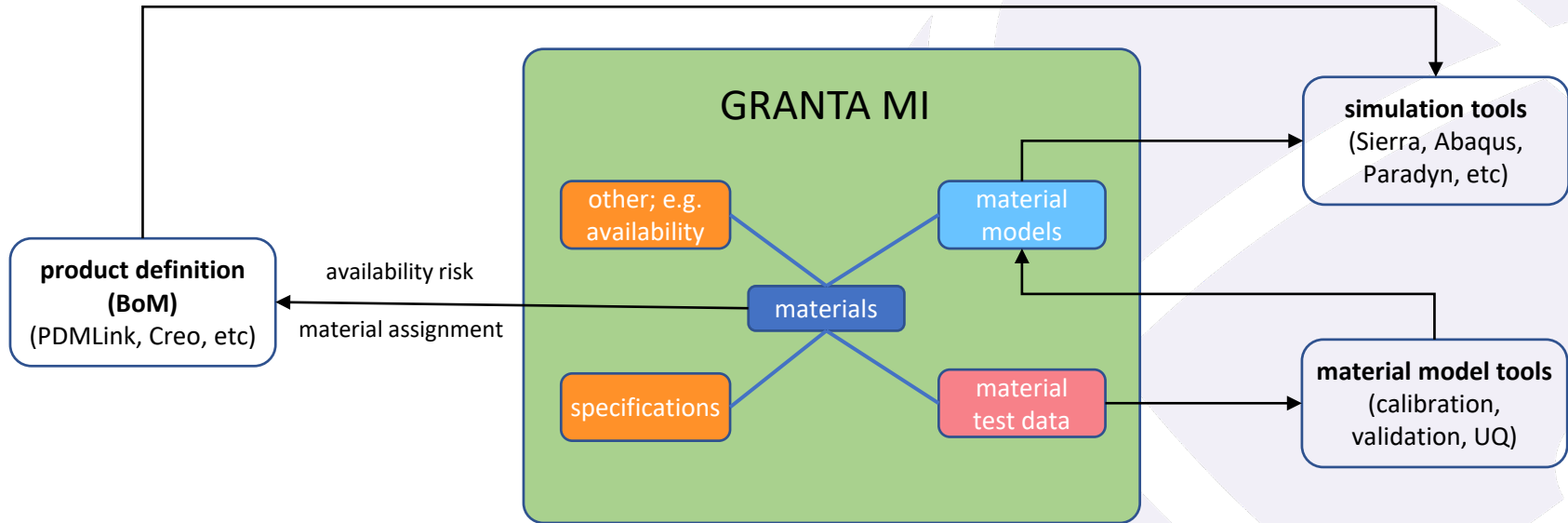
Granta stores and links many types of material information and integrates with other tools and workflows

End state: Granta will be an enterprise material data management solution

- Each site will have Granta **licenses** and **access**
- Each site will have local ('**private**') databases
- Each site may contribute to and pull from **shared** database
- Tools for **uploading** and **reporting** data may be shared
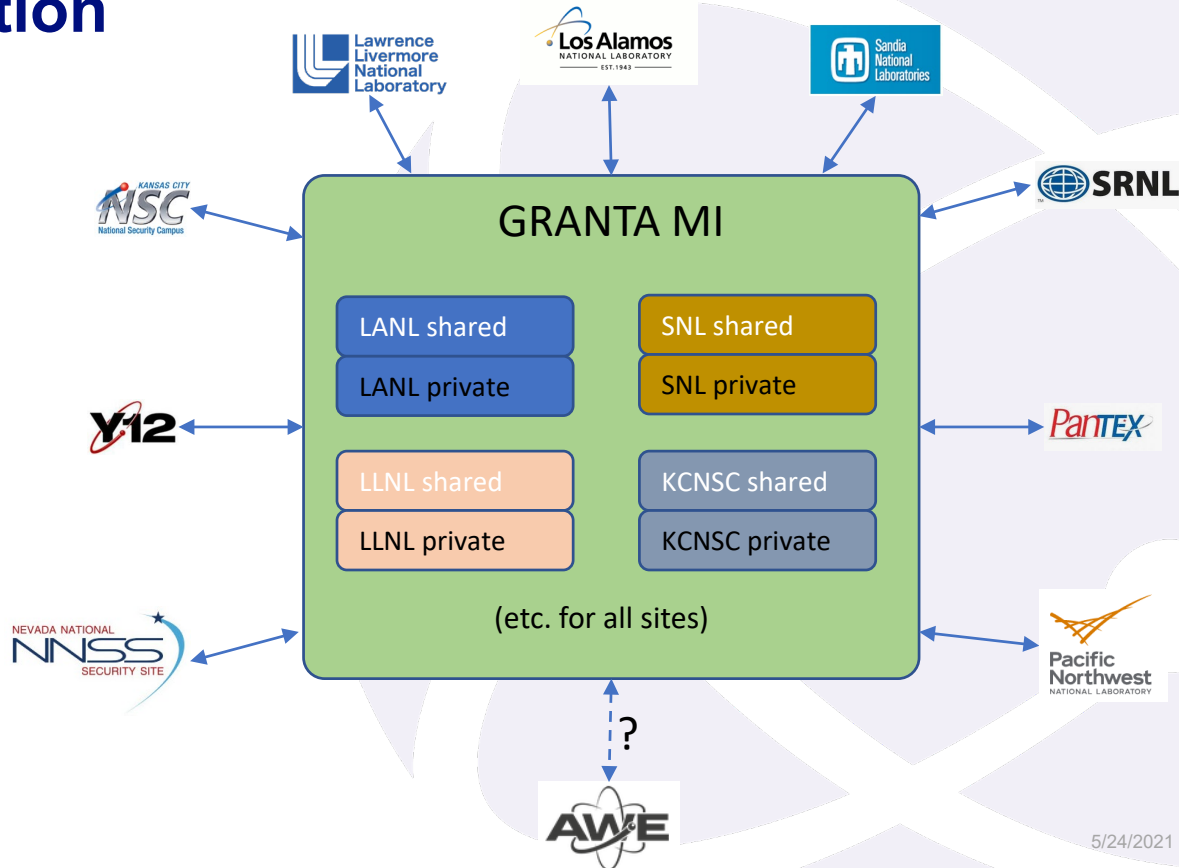
Current state: Multiple sites use Granta independently

- Currently **375 floating licenses** across all U.S. sites
- Some sites do not have production Granta instances
- The sites that have Granta instances **do not use the same schema**
  - LLNL, AWE, SNL, KCNSC, LLNL
  - Sharing data is painful
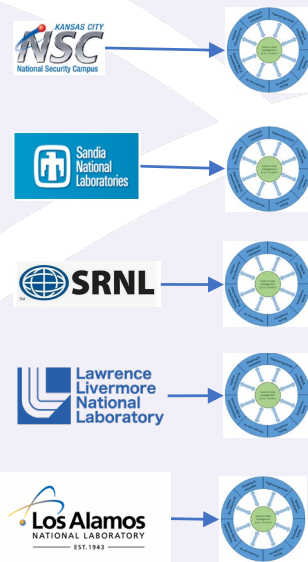 - Site-specific uploading and reporting tools are maintained
  - Use of Granta is often poorly documented
- Programs that make use of Granta include:
  - **At-Risk Materials**: uses shared classified Granta
  - **Additive Manufacturing**: uses local instances (*with schema differing between sites*)
  - **Archiving & Support**: to capture legacy data and CMMs

Each site has different:
- Schema
- Workflow
- Tools

Current state: Shared servers are not fully functional

- Classified:
  - Authentication method is 'custom'. This **doesn't allow**:
    - **upload tools** to be used at all sites
    - database **administration** at all sites
    - **integration** with Creo, Ansys, etc
    - use of **Python** STK
  - The only 'aligned' schema is for At-Risk Materials

- Unclassified:
  - No shared production server exists
  - A shared development server exists to help with schema alignment
    - Gaining access from other sites is non-trivial

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To-do: Create and document a common database schema

- Surprisingly **easy to do** – sites generally agree on schema

- Surprisingly **difficult to fund** – programs want to *use* Granta, not develop it

- **Documentation is critical** so that schema is used correctly

- Current efforts:
  - **Schema Elements** project (~0.5FTE)
    - Additive Manufacturing (AM) database Schema alignment (~0.5FTE)
  - Calibrated Material Models Working Group (CMMWG)

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To-do: AM Schema Elements project

- Funded by AM program
  - But there is much overlap with Weapons Materials Database (e.g. Tensile Testing)
- Effort: ~0.5FTE at LANL
- Development Granta instance, accessible by all sites
  - All sites can work in parallel to create and document schema
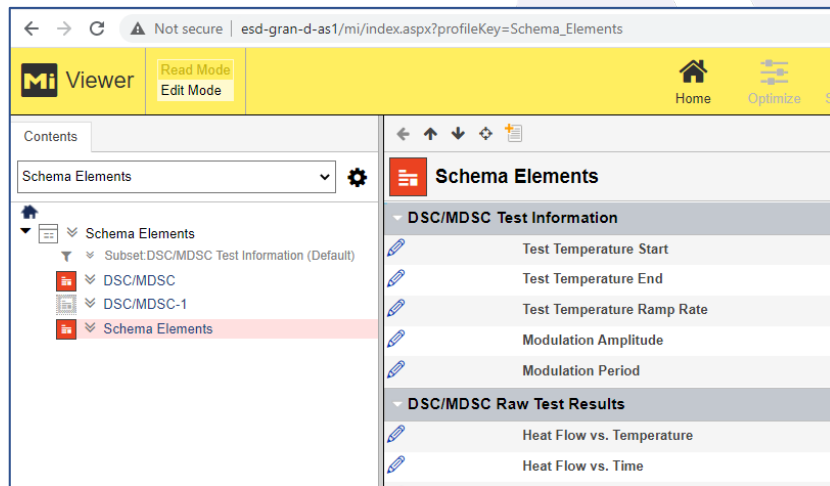
To-do: Calibrated Material Models Working Group (CMMWG)

- Proposed at 2019 Hocwog

- CMMWG has met twice:
  - SNL, October 2019
  - Virtual, November 2020

- Attendance:
  - Engineering analysts
  - Material modelers
  - Granta POCs

- Topics:
  - Material modeling methods
  - CMM database schema

Purpose

The primary purpose of the CMMWG is to provide the technical input necessary for the development of a standard calibrated material models database schema that is useful to all sites both locally and for sharing information among sites. It is not the responsibility of the CMMWG to deliver this standardized schema, but the CMMWG may be used to track and communicate progress of that deliverable.

A secondary purpose is to provide a venue for technical information exchange related to calibrated material models that may be too narrowly focused to be appropriate for other venues, such as the HOCWOG or the Nuclear Weapons Engineering Analysis Conference (NWEAC).

The topic of a standardized database schema for calibrated material models necessitates inclusion and discussion of many related topics, including but not limited to:

- Materials testing methods, results, and data types
- Component/assembly testing
- Parameter calibration methods
- Validation and verification
- Coding methods and code management

CMMWG Charter

To-do: Calibrated Material Models Working Group (cont'd)

- Topics discussed:
  - Material modeling methods:
    - Bayesian calibration
    - Uncertainty Quantification
    - Gaps in test data (e.g. intermediate strain rates)
    - Hierarchical validation
  - CMM database schema
    - 'Properties' vs. 'model parameters'
    - How to store large data (e.g. full field data)
    - 'Quality' scores for test data and CMMs
    - Integration of CMMs in Granta with:
      - Analysis codes
      - Code repos defining material model equations
    - Documenting calibration procedures

CMMWG meeting notes in SharePoint

(To read/contribute, request access to "Granta MI Materials Database" on sarape.sandia.gov)

To-do: Create, improve, and maintain shared Granta servers

- Implement OIDC authentication on classified shared server
  - LANL + LLNL + Granta are working on this
  - This will allow full functionality
    - Creo, Python, etc
- Create shared unclassified production server
  - This will allow 'master' schema to be maintained on the low side
  - This may allow some direct data sharing with AWE

Deep Dive: Storing uncertainty quantification (UQ) data for CMMs in Granta

- UQ Philosophy
  - If something is done very often, it should be made easy
    - E.g. Abaqus doesn't make the user write a subroutine for J2 plasticity – it's common so it's included
  - LANLs EABM tools were written with UQ in mind, so it is relatively easy to do
  - Storing, documenting, and retrieving UQ data in Granta needs to be 'easy'
    - UQ can be simple (e.g. "+/- 10% variation")
    - Or complicated (sampling from discrete joint distributions)
    - So we would like the option to store the data in multiple ways
    - We would like these ways connected and consistent.

Deep Dive: Storing uncertainty quantification (UQ) data for CMMs in Granta

- Nathan Miller's real-time explanation of our UQ use-case to Granta
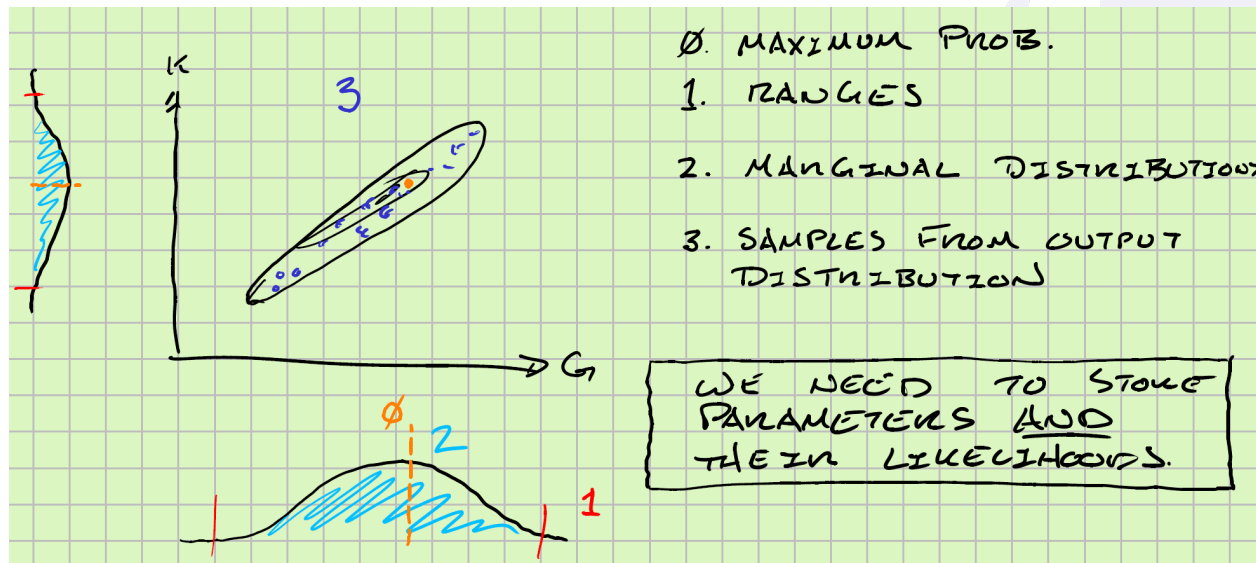
- **Level 0**: **Nominal**. This is the most likely value of a parameter
- **Level 1**: **Range**. The parameter falls between these two values. E.g. "+/- 10%"
- **Level 2**: **Marginal Distribution**. The parameter is described by a known independent distribution (or samples from a known independent distribution)
- **Level 3**: **Joint Distribution**. The likelihood of a value for parameter G depends on the value of parameter K.

If we populate one level, we want all levels populated (with a user-defined set of assumptions)

Summary

- End state – shared schema, and some shared data, across all sites
- Current state – some sites are using Granta, but they're doing it differently
- To-do – align schema, resolve shared server difficulties
- Deep dive – we've drafted a method of storing UQ CMM data in Granta
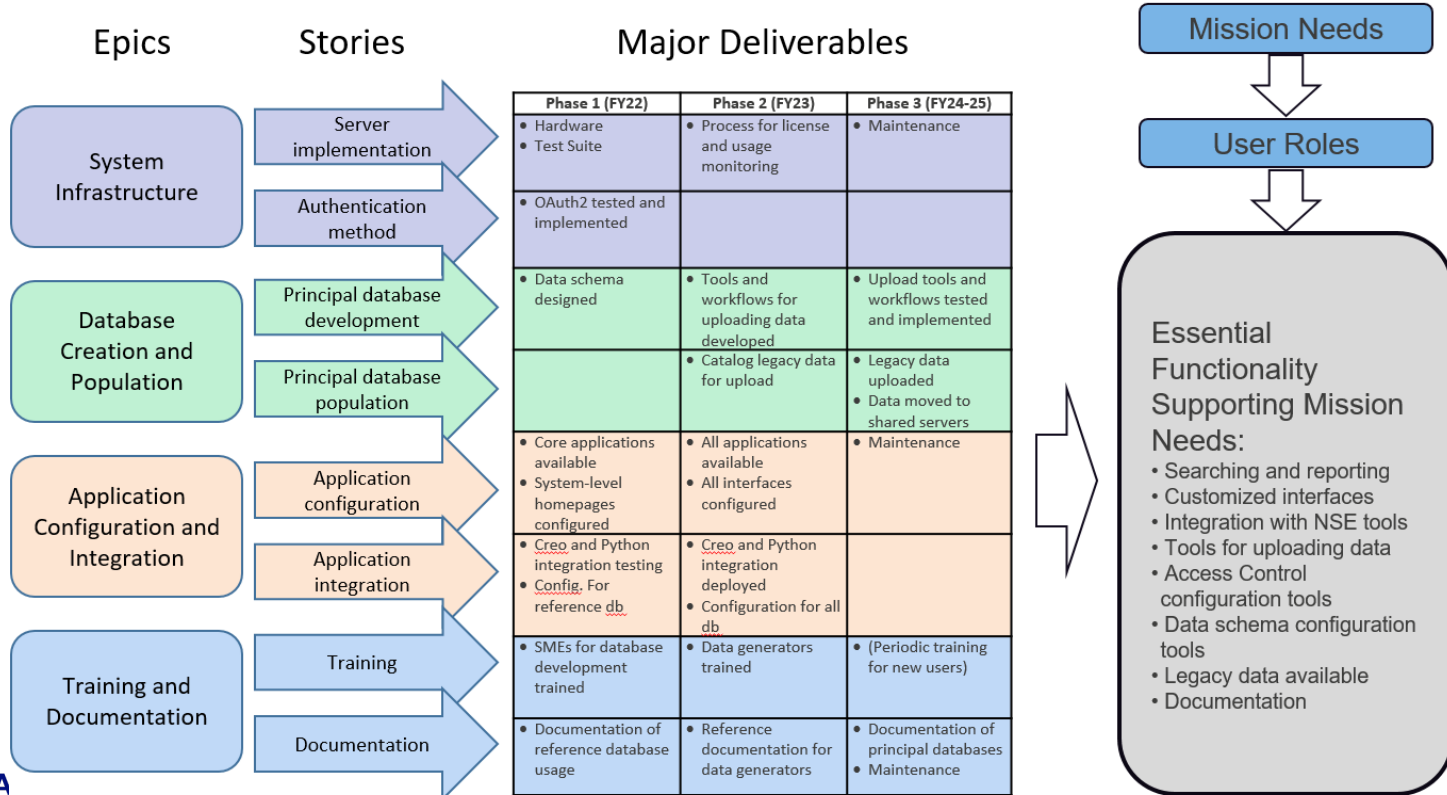
There are many facets of this project where you can be involved

Questions, comments & discussion

A development plan for enterprise Granta implementation had been drafted

| Epics | Stories | Major Deliverables |
| | | Phase 1 (FY22) | Phase 2 (FY23) | Phase 3 (FY24-25) |

Epics:
- System Infrastructure
- Database Creation and Population
- Application Configuration and Integration
- Training and Documentation

Stories:
- Server implementation
- Authentication method
- Principal database development
- Principal database population
- Application configuration
- Application integration
- Training
- Documentation

Major Deliverables:

	Phase 1 (FY22)	Phase 2 (FY23)	Phase 3 (FY24-25)
Server implementation	• Hardware • Test Suite	• Process for license and usage monitoring	• Maintenance
Authentication method	• OAuth2 tested and implemented		
Principal database development	• Data schema designed	• Tools and workflows for uploading data developed	• Upload tools and workflows tested and implemented
Principal database population		• Catalog legacy data for upload	• Legacy data uploaded • Data moved to shared servers
Application configuration	• Core applications available • System-level homepages configured	• All applications available • All interfaces configured	• Maintenance
Application integration	• Creo and Python integration testing • Config. For reference db	• Creo and Python integration deployed • Configuration for all db	
Training	• SMEs for database development trained	• Data generators trained	• (Periodic training for new users)
Documentation	• Documentation of reference database usage	• Reference documentation for data generators	• Documentation of principal databases • Maintenance

Mission Needs → **User Roles** →

Essential Functionality Supporting Mission Needs:
- Searching and reporting
- Customized interfaces
- Integration with NSE tools
- Tools for uploading data
- Access Control configuration tools
- Data schema configuration tools
- Legacy data available
- Documentation

Vision is for an aligned, well-documented, and highly effective materials data management solution